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Model two-dimensional liquid ^{3}He–^{4}He mixture within the self-consistent field approximation

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Abstract

In this paper we use the self-consistent scheme proposed by Singwi, Tosi, Land and Sjölander (STLS) to study a model two-component fermion–boson system (^{3}He–^{4}He mixture) in two dimensions. We calculate the partial static structure factors and effective potentials, given a model bare interaction with hard-core plus an attractive tail. We study the dependence of these quantities on the ^{3}He fraction in the mixture. Collective modes for the mixture are also discussed.

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Keywords: Fermion–boson system; Liquid ^{3}He–^{4}He; Two-dimensional system; Self-consistent field

1. Introduction

Ng and Singwi [1–3] in a series of papers have studied a model Fermi liquid interacting via a hard-core repulsive potential and an attractive tail within the self-consistent field approach. This simple model remarkably reproduced some key features of both the normal and spin-polarized liquid ^{3}He providing insight into the nature of strongly coupled Fermi systems. A similar investigation for a two-dimensional Fermi liquid was performed by da Silveira et al. [4]. These calculations along with some earlier reports [5–7] have shown that the self-consistent field method of Singwi, Tosi, Land, and Sjölander (STLS) [8,9] originally devised to treat the short-range correlation effects in Coulomb liquids (interacting via the long-range $1/r$ potential) is also capable of handling systems interacting via short-range potentials. A qualitative agreement was found between the calculated and the experimental results. Recently, Nafari and Doroudi [10,11] have used the realistic inter-atomic potential to study the ground state properties of liquid ^{3}He (in three and two dimensions) within the STLS scheme, improving the level of agreement with experiments.

In this work we apply the method of Ng and Singwi [1–3] to a two-dimensional (2D) liquid ^{3}He–^{4}He mixture interacting via a repulsive hard-core potential. There are several motivations to study the two-component (fermion–boson) extension of the self-consistent field approximation. A

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dilute solution of ^{3}He atoms in liquid ^{4}He forms a fascinating quantum liquid (both in the bulk and as film structures) as an example of interacting fermion–boson mixture. In a recent work [12], we have extended the STLS self-consistent field method for a fermion–boson mixture interacting with hard-core potentials to obtain qualitative agreement with the realistic ^{3}He–^{4}He mixtures in the bulk. ^{3}He atoms adsorbed on the free surface or films of liquid ^{4}He are of interest [13–15]. Even though it is very difficult to achieve experimentally a 2D liquid ^{3}He–^{4}He mixture because of the formation of the Andreev state [16] and the localization properties of ^{3}He atoms [17], we consider an idealized model system. Such a model has recently been studied by Um et al. [18]. Within the hypernetted chain scheme and by Grisenti and Reatto [19] using a variational Monte Carlo method. It would be interesting to obtain a qualitative understanding of the salient features of these idealized 2D systems. Another source of motivation is the fermion–boson mixture of atomic gases in trap potentials [20,21] which is of recent interest because it provides a testing ground for interaction and statistical effects. Our calculations could be a reference for comparison when the effects of external potentials are taken into account. There has been many attempts to understand the ground state energy, correlation functions, collective excitations and single-particle properties of bulk liquid ^{3}He–^{4}He mixtures using a variety of methods [22–26]. Thus, we can compare our results with those in the bulk to assess the dimensionality effects.

Our chief aim in this work is to see how well the ground state properties of a 2D liquid ^{3}He–^{4}He mixture are described within the STLS approximation scheme. To facilitate our discussion we employ a model hard-core repulsive potential with an attractive tail. The self-consistent field method (or the STLS approximation) renormalizes the bare hard-core potentials to yield reasonable ground state structure factors. We also study the effect of an attractive tail in the bare potential on the partial static structure factors, effective interactions, and collective excitation modes. We find that the STLS method provides a reasonable qualitative description of 2D liquid ^{3}He–^{4}He mixtures which may be useful in the analysis of static and dynamical properties. In the rest of this paper, we first provide a brief background on the self-consistent field method as applied to a multi-component system, and then discuss our results for the 2D liquid ^{3}He–^{4}He mixtures. We conclude with a short summary.

2. Model and theoretical framework

The multi-component generalization of the STLS theory is based on the approximation that the fluctuations in the density (of say the αth component) within the linear response theory is written as

$$\delta n_\alpha(q,\omega) = \sum_\beta \chi_{\alpha\beta}(q,\omega) V_\beta^{\mathrm{ext}}, \tag{1}$$

where $\tilde{\chi}$ is the density–density response matrix, and V_α^{ext} is the external perturbing field. In the self-consistent field approach of Singwi et al. [8,9] the response of the system to an external potential is expressed as

$$\delta n_\alpha = \chi_\alpha^0(q,\omega)\left[V_\alpha^{\mathrm{ext}} + \sum_\beta V_{\alpha\beta}^{\mathrm{eff}}(q)\delta n_\beta \right], \tag{2}$$

where $\chi_\alpha^0(q,\omega)$ is the response of the non-interacting αth component. Combining the above equations, we obtain the STLS expression for the density–density response function of the multi-component system

$$\chi_{\alpha\beta}^{-1}(q,\omega) = [\chi_\alpha^0(q,\omega)]^{-1}\delta_{\alpha\beta} - V_{\alpha\beta}^{\mathrm{eff}}(q). \tag{3}$$

The effective interparticle interactions within the STLS scheme are related to the pair-distribution functions $g_{\alpha\beta}(r)$ through [2,3]

$$V_{\alpha\beta}^{\mathrm{eff}}(r) = -\int_r^\infty \mathrm{d}r'\, g_{\alpha\beta}(r')\frac{\mathrm{d}V}{\mathrm{d}r'}, \tag{4}$$

where $V(r)$ is the bare interaction potential for helium atoms, $g_{\alpha\beta}(r)$ is the partial pair correlation function for the two-dimensional system, related to the static structure factors $S_{\alpha\beta}(q)$ by

$$g_{\alpha\beta}(r) = 1 + \frac{1}{(n_\alpha n_\beta)^{1/2} 2\pi}\int_0^\infty \mathrm{d}q\, qJ_0(qr)[S_{\alpha\beta}(q) - \delta_{\alpha\beta}], \tag{5}$$

in which $J_0(x)$ is the zeroth-order Bessel function. We calculate $S_{\alpha\beta}(q)$ with the aid of the fluctuation–dissipation theorem

$$S_{\alpha\beta}(q) = -\frac{1}{\pi(n_\alpha n_\beta)^{1/2}}\int_0^\infty \mathrm{d}\omega\, \chi_{\alpha\beta}(q, \mathrm{i}\omega), \tag{6}$$

in which $\chi_{\alpha\beta}(q, \mathrm{i}\omega)$ are the density–density response functions evaluated on the imaginary frequency axis. We consider the model bare potential in the form

$$V(r) = \begin{cases} V_0, & r < a_0, \\ 0, & a_0 < r, \end{cases} \tag{7}$$

where V_0 is the strength of the potential and a_0 is the hard-core radius. By substituting Eq. (7) in Eq. (4) and taking the Fourier transform of the hard-core ($V_0 \to \infty$) potential we obtain [4]

$$V^{\mathrm{eff}}_{\alpha\beta}(q) = 2\pi \frac{V_0 g_{\alpha\beta}(a_0)}{q} J_1(qa_0), \tag{8}$$

where $J_1(x)$ is the first-order Bessel function. For the hard-core bare potential Eq. (5) gives three non-linear equations. We have solved the above equations for the unknown parameters $V_0 g_{\alpha\beta}(a_0)$ for various densities and ^{3}He fractions. The realistic potential between helium atoms does not only has a steep hard core but it also has an attractive tail. To this purpose it is possible to consider a model potential

$$V(r) = \begin{cases} V_0, & r < a_0, \\ -\varepsilon, & a_0 < r < a_1, \\ 0, & a_1 < r, \end{cases} \tag{9}$$

where ε is the depth of the potential well and a_1 is its width. The above model potential yields the effective interaction [4]

$$V^{\mathrm{eff}}_{\alpha\beta}(q) = \frac{2\pi}{q}[(V_0 + \varepsilon) g_{\alpha\beta}(a_0) J_1(qa_0) - \varepsilon a_1 g_{\alpha\beta}(a_1) J_1(qa_1)], \tag{10}$$

where $\varepsilon g_{\alpha\beta}(a_1)$ are extra unknown parameters to be determined. The number of equations to be self-consistently solved in this case are doubled.

The self-consistent field method set out above has the general structure as the random-phase approximation (RPA) with bare interactions replaced by effective interactions. Since the effective interactions are purely static, and no self-energy effects are included in the response functions, the model leaves no room for the multi-particle effects. This should not affect the static structure factors calculated in this work in a significant way, but would be important for the dynamical properties.

3. Numerical Results

In our study we consider ^{3}He absorbed on a thin film of ^{4}He forming a two-dimensional ^{3}He–^{4}He mixture. The total number of helium atoms in the sample with area A is given by $N = N_3 + N_4$, in terms of the number of ^{3}He and ^{4}He atoms, and the corresponding particle density is $N/A = n = n_3 + n_4$. Denoting the fraction of ^{3}He atoms in the mixture by x, we have $n_3 = xn$ and $n_4 = (1 - x)n$. We scale all lengths by the hard-core radius a_0, and the energies by the effective Rydberg $1/(2\mu a_0^2)$ (we take $\hbar = 1$) where $\mu = m_3 m_4/(m_3 + m_4)$ is the reduced mass. For convenience the density is expressed in terms of $n_0 = 1/(\pi a_0^2)$. For ^{3}He atoms in the mixture we define the Fermi wave vector $k_{\mathrm{F}} a_0 = [(2\pi)x(n/n_0)]^{1/2}$.

We begin discussing our results with the solution of self-consistent equations [i.e. Eqs. (5) and (6)]. Fig. 1 shows $V_0 g_{\alpha\beta}(a_0)$ as a function of density for $x = 0.05$. The general behavior is similar for the two model potentials (with and without the attractive tail) and also similar to the three dimensional case [12], where we have a broad peak around $n/n_0 = 0.8$. In the case of normal and spin-polarized fluid ^{3}He, Ng and Singwi [1–3] were not able to find convergent solutions to the nonlinear equations beyond a certain density and suggested the interpretation of freezing transition. We were able to find stable solutions for $n/n_0 \lesssim 1.5$. Here, we take $a_0 \approx 2.5\,\text{Å}$ and use $n/n_0 \approx 0.8$, to have equilibrium density [18,19] $n \sim 0.04\,\text{Å}^{-2}$.

In Fig. 2 we compare our results for the 2D ^{3}He–^{4}He mixture static structure factors $S_{\alpha\beta}(q)$ with those in a 3D mixture. The enhancement of the structure factor $S_{44}(q)$ is very clear in 2D compared to the 3D case for the same ^{3}He fraction and density [12]. Due to the diluteness of ^{3}He atoms in the mixture $S_{33}(q)$ shows very little structure (as in

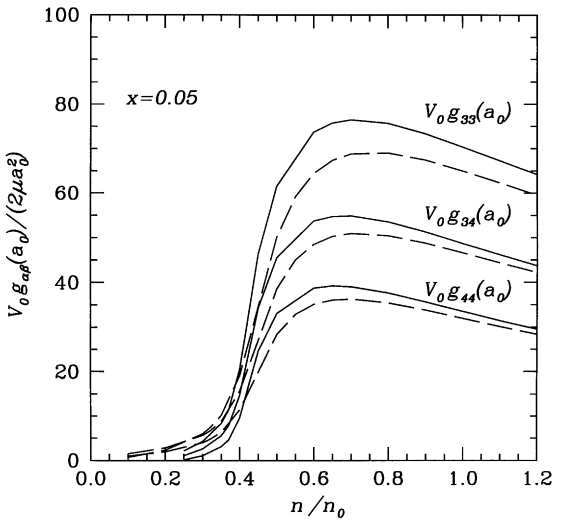

Fig. 1. The density dependence of the coefficients $V_0 g_{\alpha\beta}(a_0)$ with (solid lines) and without (dashed lines) attractive tail in the bare potential at $x = 0.05$. For the attractive tail part, we took $\varepsilon \approx 5\,\mathrm{K}$ and $a_1/a_0 = 2$.

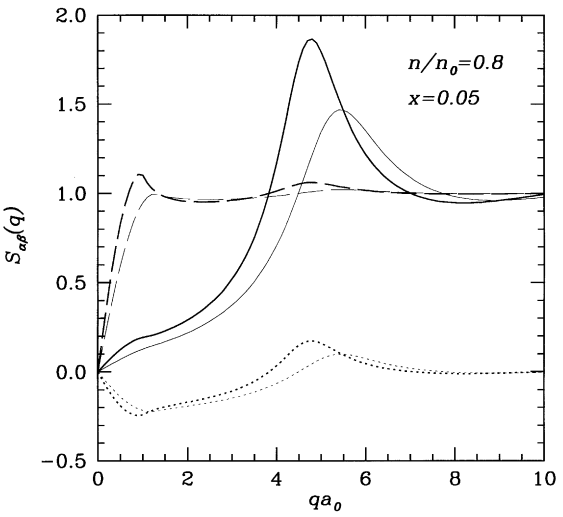

Fig. 2. The partial static structure factors for liquid ^{3}He–^{4}He mixture in 2D (thick lines) and 3D (thin lines) at $x = 0.05$ and $n/n_0 = 0.8$, considering the hard-core potential only. The solid, dashed, and dot–dashed lines refer to $S_{44}(q)$, $S_{33}(q)$, and $S_{34}(q)$, respectively.

the 3D case [12]). The effect of the attractive tail in the bare potential is displayed in Fig. 3. The structure factors $S_{33}(q)$ and $S_{34}(q)$ are rather insensitive to the attractive part, since we have a dilute

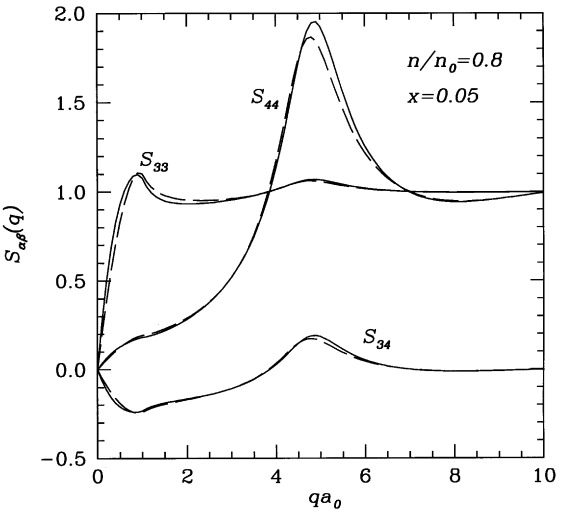

Fig. 3. The comparison of partial structure factors $S_{\alpha\beta}(q)$ in 2D liquid ^{3}He–^{4}He mixture with (solid lines) and without (dashed lines) attractive tail in the bare potential at $x = 0.05$ and $n/n_0 = 0.8$. For the attractive tail part, we took $\varepsilon \approx 5\,\mathrm{K}$ and $a_1/a_0 = 2$.

mixture. The peak height and position of $S_{44}(q)$ slightly increases and moves to the large q direction. Similar effects were also seen for mixtures in 3D. The dependence on the ^{3}He fraction of partial static structure factors are shown in Fig. 4. Increase in the ^{3}He fraction x affects $S_{44}(q)$ in the long wavelength region only (Fig. 4a) and increases the peaks values for $S_{33}(q)$ and $S_{44}(q)$ (cf. Fig. 4b and c).

Once the parameters $V_0 g_{\alpha\beta}(a_0)$ and $\varepsilon g_{\alpha\beta}(a_1)$ are known we readily obtain the resulting effective interactions $V^{\mathrm{eff}}_{\alpha\beta}(q)$ within our model. Fig. 5 displays the effective interactions between the 2D ^{3}He and ^{4}He atoms. We observe that the attractive part of the potential does not influence the resulting effective interactions $V^{\mathrm{eff}}_{\alpha\beta}(q)$ very dramatically except for the long wavelength region where it is typically larger compared to the pure hard-core results.

The collective excitations are determined by solving for the roots of the determinant of the dynamic response matrix $\mathrm{Det}[\chi_{\alpha\beta}(q,\omega)^{-1}] = 0$, which yields

$$1 - V^{\mathrm{eff}}_{33}(q)\chi^0_3(q,\omega) - V^{\mathrm{eff}}_{44}(q)\chi^0_4(q,\omega) + [V^{\mathrm{eff}}_{33}(q)V^{\mathrm{eff}}_{44}(q) - (V^{\mathrm{eff}}_{34}(q))^2]\chi^0_3(q,\omega)\chi^0_4(q,\omega) = 0. \quad (11)$$

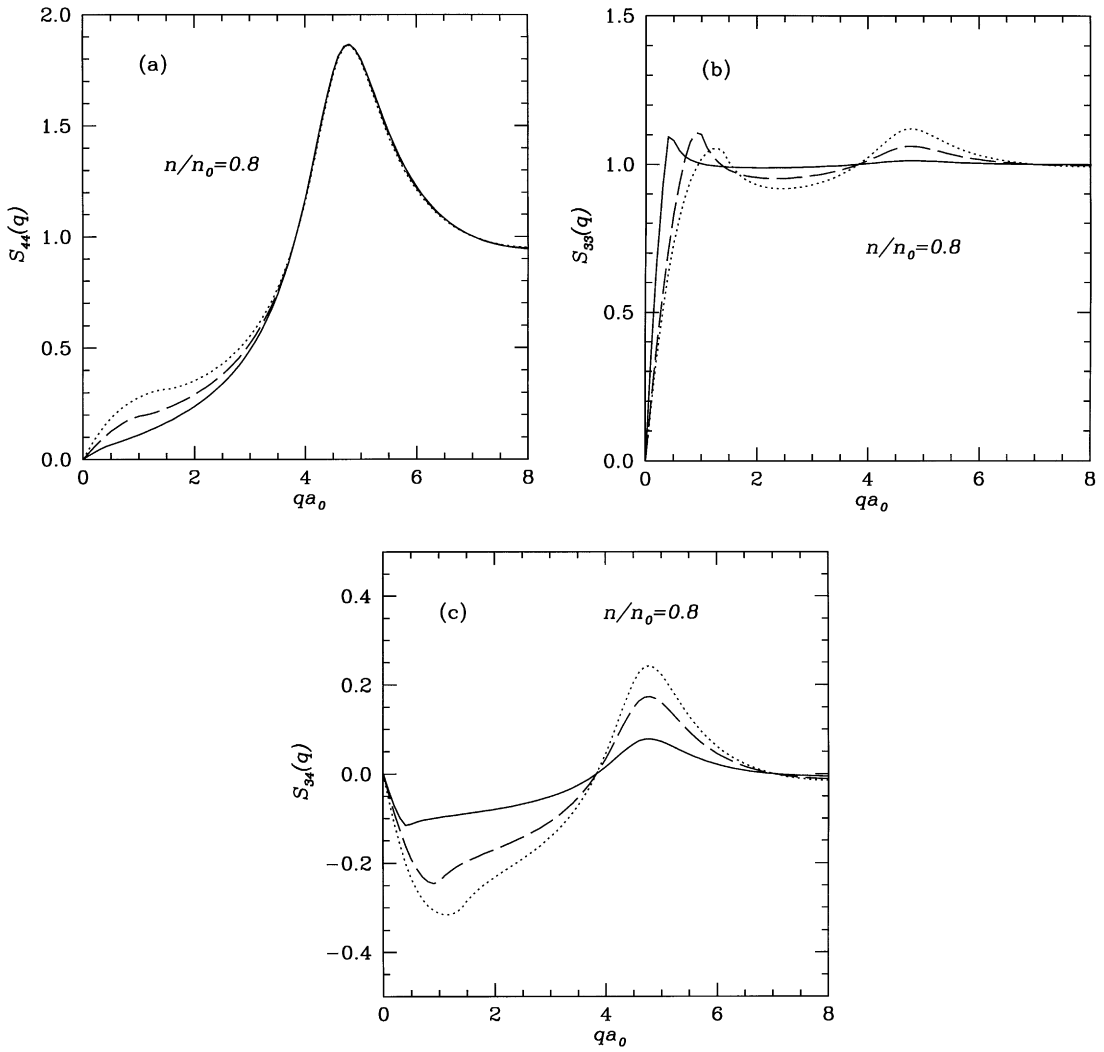

Fig. 4. (a) The static structure factor $S_{44}(q)$ for liquid ^{3}He–^{4}He mixture without attractive tail in the bare potential at $n/n_0 = 0.8$ and $x = 0.01$ (solid line), $x = 0.05$ (dashed line) and $x = 0.1$ (dotted line). (b) The static structure factor $S_{33}(q)$ at $n/n_0 = 0.8$ and $x = 0.01$ (solid line), $x = 0.05$ (dashed line) and $x = 0.1$ (dotted line). (c) The static structure factor $S_{34}(q)$ at $n/n_0 = 0.8$ and $x = 0.01$ (solid line), $x = 0.05$ (dashed line) and $x = 0.1$ (dotted line).

We investigate the collective excitations of the liquid ^{3}He–^{4}He mixture within the mean-spherical approximation (MSA) [24] for the ^{3}He component. In the MSA, the particle-hole continuum and the collective mode of a Fermi system (described by the usual Lindhard function) is replaced by a single effective collective mode excitation. More specifically, the non-interacting response of ^{3}He atoms is given by $\chi_3^0(q,\omega = 2n_3\varepsilon_q^{(3)}/[(\omega + i\eta)^2 + (\varepsilon_q^{(3)}/S_0(q))^2]$, where $\varepsilon_q^{(3)} = q^2/2m_3$ and $S_0(q)$ is the 2D Hartree–Fock static structure factor which is given as

$$S_0(q) = \begin{cases} \left(\frac{2}{\pi}\right)\sin^{-1}\left(\frac{q}{2k_F}\right) + \left(\frac{q}{\pi k_F}\right)\left[1 - \left(\frac{q}{2k_F}\right)^2\right]^{1/2}, & q < 2k_F, \\ 1, & q > 2k_F. \end{cases} \quad (12)$$

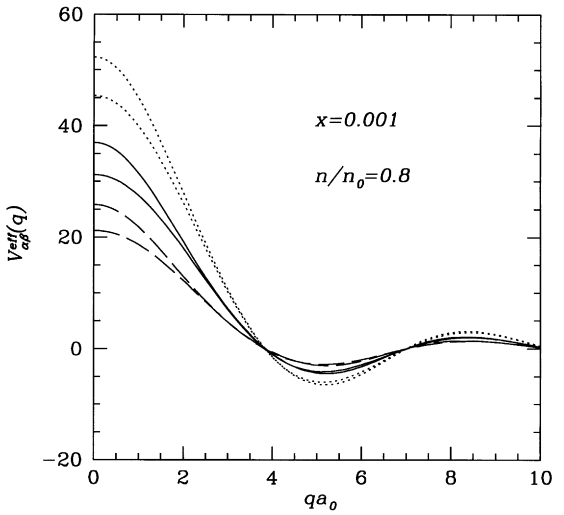

Fig. 5. The effective interactions $V_{44}^{\rm eff}(q)$ (dashed line), $V_{33}^{\rm eff}(q)$ (dotted line), and $V_{34}^{\rm eff}(q)$ (solid line) for 2D liquid ^{3}He–^{4}He mixture at $x = 0.001$ and $n/n_0 = 0.8$. Upper curves near $q \approx 0$ for each $V_{\alpha\beta}^{\rm eff}(q)$ are with the attractive tail in the bare potential. Lower ones correspond to the hard core bare potential only. For the attractive tail part, we took $\varepsilon \approx 5$ K and $a_1/a_0 = 2$.

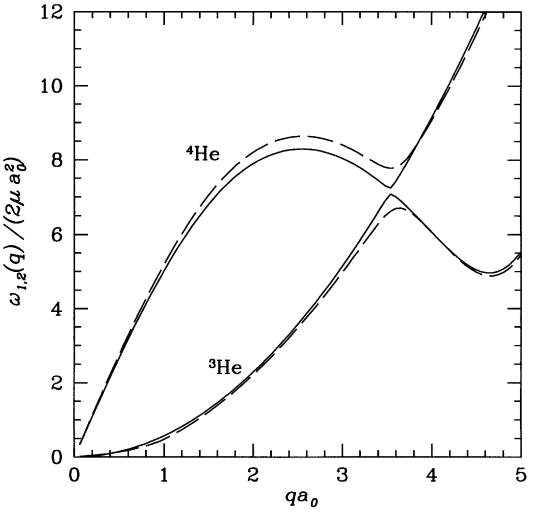

Fig. 6. The collective modes for liquid ^{3}He–^{4}He mixture at $n/n_0 = 0.8$ and $x = 0.001$ (solid line) and $x = 0.05$ (dashed line) for the full bare potential (the hard core and the attractive tail).

Using the response function of the non-interacting Bose systems given by $\chi_4^0(q,\omega) = 2n_4\varepsilon_q^{(4)}/[(\omega + i\eta)^2 - (\varepsilon_q^{(4)})^2]$, where $\varepsilon_q^{(4)} = q^2/2m_4$, in Eq. (11), we obtain the collective mode energies

$$\omega_{1,2}(q) = [\tfrac{1}{2}(\psi_{33} + \psi_{44}) \pm \tfrac{1}{2}[(\psi_{33} - \psi_{44})^2 + 4\psi_{34}]^{1/2}]^{1/2}, \quad (13)$$

where $\psi_{33} = [\varepsilon_q^{(3)}/S_0(q)]^2 + 2n_3\varepsilon_q^{(3)}V_{33}^{\rm eff}$, $\psi_{44} = [\varepsilon_q^{(4)}]^2 + 2n_4\varepsilon_q^{(4)}V_{44}^{\rm eff}$, and $\psi_{34} = 2n_3\varepsilon_q^{(3)}2n_4\varepsilon_q^{(4)}[V_{34}^{\rm eff}]^2$. The MSA is similar to the binary–boson approximation [27,28] in which the ^{3}He response function $\chi_3^0(q,\omega)$ is approximated by the Bogoliubov form as for ^{4}He component. In Fig. 6 we show the collective modes within the MSA for a 2D liquid ^{3}He–^{4}He mixture at $n/n_0 = 0.8$, and two different ^{3}He fractions. We find two discrete modes, a phonon–roton branch corresponding to ^{4}He atoms (upper curves), and a second branch corresponding to ^{3}He atoms (lower curves). The ^{3}He excitations show a dip similar to the roton minimum which can be regarded as a mode coupling effect. A similar analysis [12,24–26] for bulk ^{3}He–^{4}He mixtures suggests that in the long-wavelength region the upper and lower collective modes may be identified as the second and zeroth sound modes. We point out that including an attractive tail modifies the dispersion relations slightly, around the roton minimum for ^{4}He mode and beyond the dip structure for ^{3}He mode. Our calculations indicate that with increasing ^{3}He fraction x, the modes separate. Finally, we note that associating the collective mode dispersions with ^{3}He and ^{4}He become less clear [24–26] for larger wave vectors, i.e. $qa_0 \gtrsim 3$.

4. Summary

In this work, we considered an idealized model of 2D liquid ^{3}He–^{4}He mixtures. Starting from a hard core plus an attractive tail type of bare interaction between the helium atoms, we employed the STLS scheme to calculate the partial structure factors and the effective interactions in the mixture. We found that in general the structure factors are enhanced compared to the 3D counterparts. That the STLS scheme can be used to study the ground state properties of systems of fermion–boson mixtures is demonstrated in a 2D model. Our results could

complement the more sophisticated approaches such as the hypernetted chain approximation [18] to obtain a qualitative understanding. Finally, our calculations may be improved by including the self-energy corrections describing multi-particle effects.

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